

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
 Data File : BF112757.D
 Acq On : 28 Feb 2019 12:54
 Operator : JU/SJ
 Sample : K1596-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-14

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.934	477	484	492	rVB	48320	63622	1.76%	0.174%
2	5.351	550	555	558	rBV	3524974	3522361	97.34%	9.616%
3	6.375	724	729	733	rBV	3746294	3578667	98.90%	9.770%
4	6.510	748	752	756	rBV	3921975	3618455	100.00%	9.879%
5	6.745	788	792	795	rBV	1197932	1023568	28.29%	2.794%
6	6.898	814	818	822	rBV	3098810	2676149	73.96%	7.306%
7	7.298	882	886	889	rBV	2379945	2188044	60.47%	5.974%
8	8.022	1006	1009	1013	rBV	1364387	1156472	31.96%	3.157%
9	9.098	1188	1192	1195	rBV	3655833	2997009	82.83%	8.182%
10	9.192	1205	1208	1211	rBV2	49113	46756	1.29%	0.128%
11	9.486	1256	1258	1261	rBV	253732	216550	5.98%	0.591%
12	9.633	1279	1283	1286	rBV	95768	99780	2.76%	0.272%
13	9.769	1302	1306	1310	rBV	1199226	1163457	32.15%	3.176%
14	9.975	1339	1341	1345	rVB2	63007	60706	1.68%	0.166%
15	10.439	1416	1420	1423	rBV3	34074	41627	1.15%	0.114%
16	10.551	1435	1439	1443	rBV	2214222	2187691	60.46%	5.973%
17	10.686	1459	1462	1464	rBV3	52641	61202	1.69%	0.167%
18	10.922	1499	1502	1505	rBV3	68944	68514	1.89%	0.187%
19	10.998	1513	1515	1521	rVB4	28989	43476	1.20%	0.119%
20	11.169	1541	1544	1547	rVB	50380	48582	1.34%	0.133%
21	11.251	1554	1558	1560	rBV	1298571	1252008	34.60%	3.418%
22	11.269	1560	1561	1565	rVB	467852	336361	9.30%	0.918%
23	11.322	1565	1570	1573	rBV2	195347	180730	4.99%	0.493%
24	11.357	1573	1576	1582	rBV6	25865	44867	1.24%	0.122%
25	11.474	1594	1596	1600	rVB	61221	56699	1.57%	0.155%
26	11.751	1641	1643	1645	rBV	65566	47210	1.30%	0.129%
27	11.786	1645	1649	1653	rBV2	686423	799467	22.09%	2.183%
28	11.857	1658	1661	1664	rBV	135039	147280	4.07%	0.402%
29	12.045	1690	1693	1694	rBV	65940	62830	1.74%	0.172%
30	12.245	1725	1727	1730	rVB4	53165	42785	1.18%	0.117%
31	12.298	1733	1736	1739	rVV3	141494	124310	3.44%	0.339%
32	12.457	1759	1763	1766	rBV	897753	789185	21.81%	2.155%
33	12.569	1780	1782	1787	rBV	406902	426728	11.79%	1.165%
34	12.680	1796	1801	1804	rBV	841224	817069	22.58%	2.231%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	12.833	1823	1827	1830	rBV	3533509	3091039	85.42%	8.439%
36	13.080	1866	1869	1871	rBV2	123136	114623	3.17%	0.313%
37	13.116	1872	1875	1877	rBV	127346	141848	3.92%	0.387%
38	13.733	1978	1980	1991	rVB5	249266	352667	9.75%	0.963%
39	13.874	2000	2004	2007	rBV2	1680502	1873227	51.77%	5.114%
40	13.898	2007	2008	2012	rVB	346140	273021	7.55%	0.745%
41	15.292	2242	2245	2248	rVB	714069	791679	21.88%	2.161%

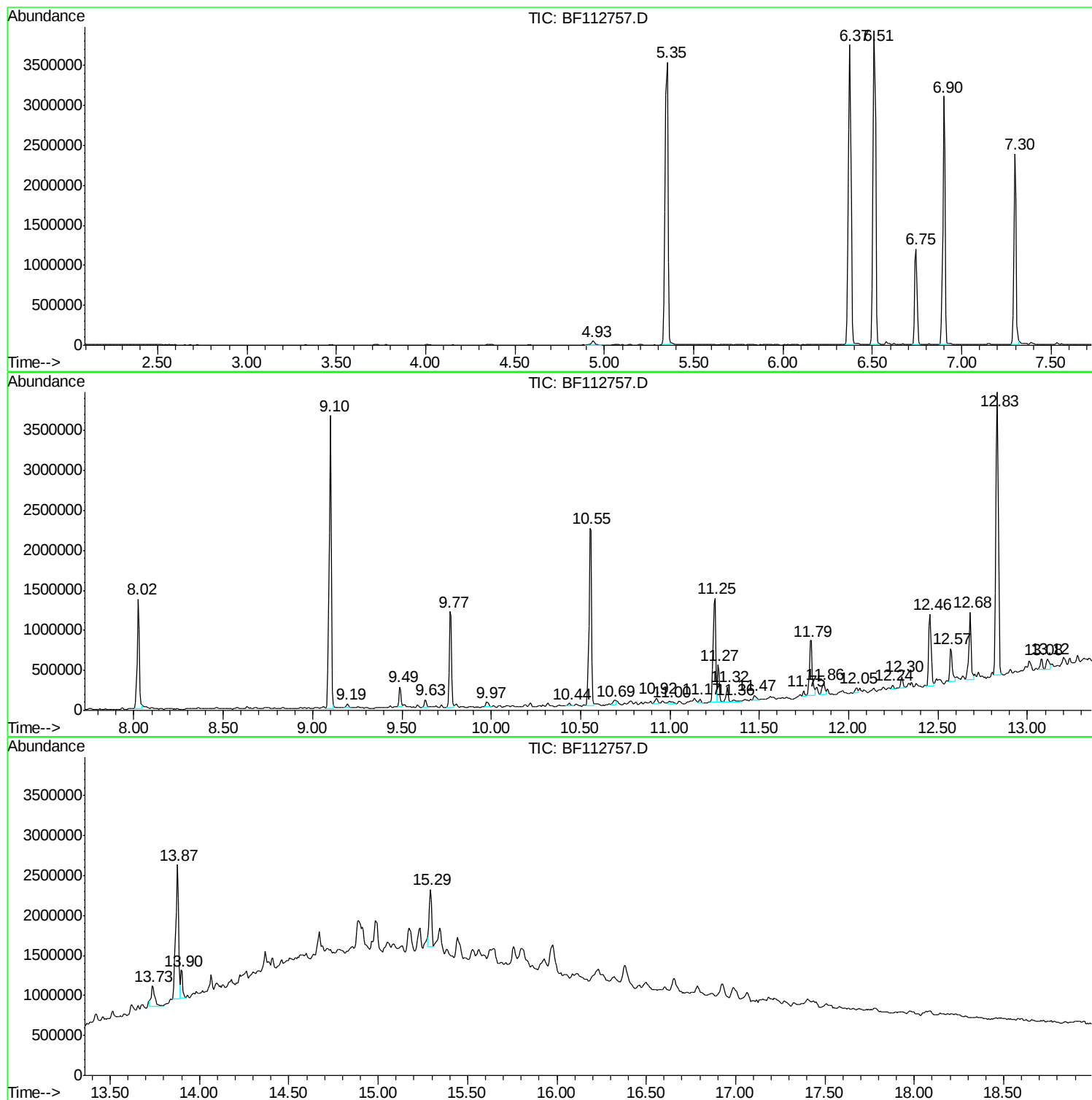
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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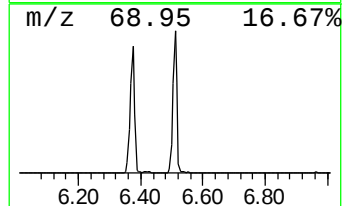
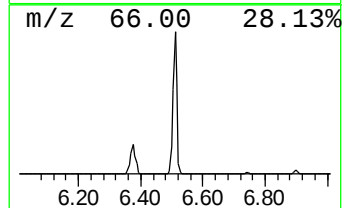
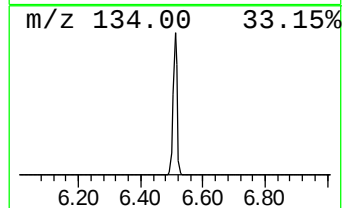
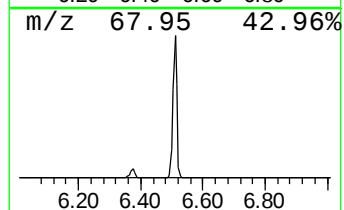
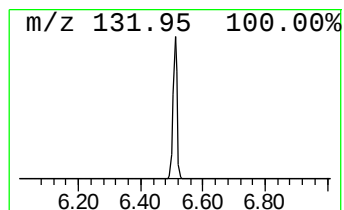
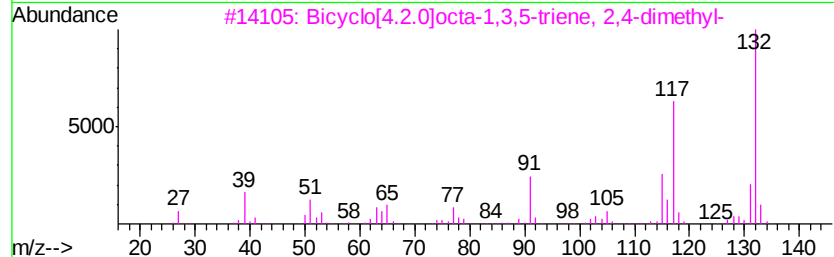
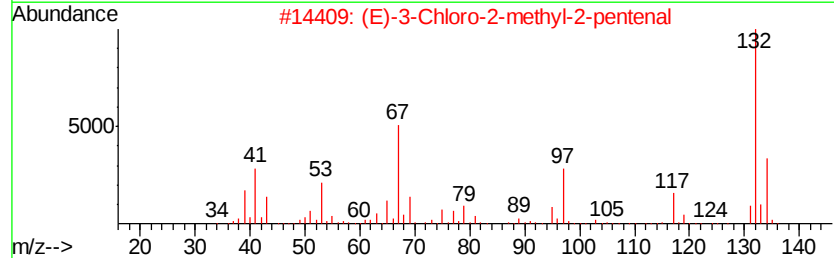
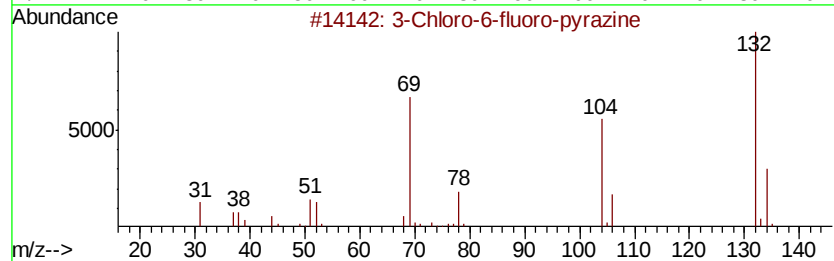
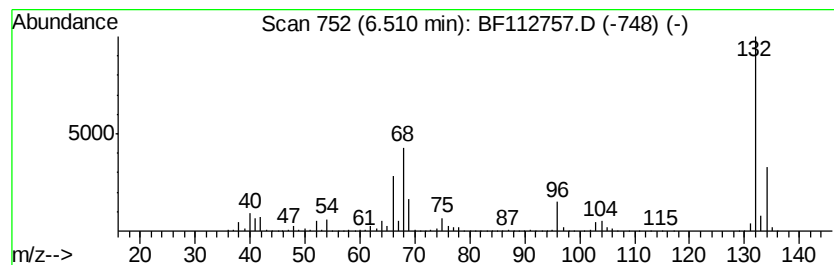
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	70.70 ng	3618460	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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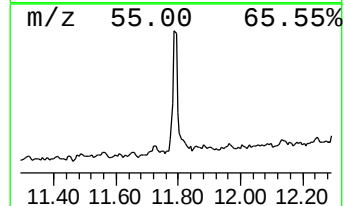
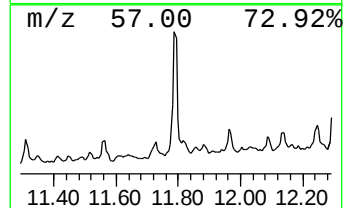
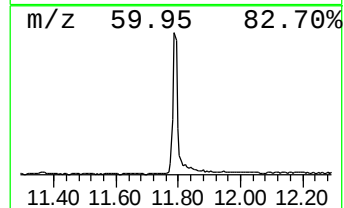
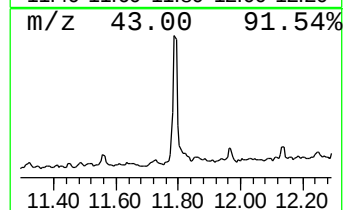
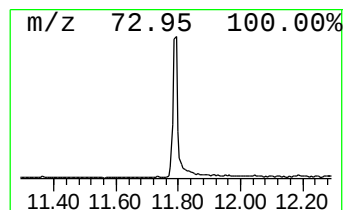
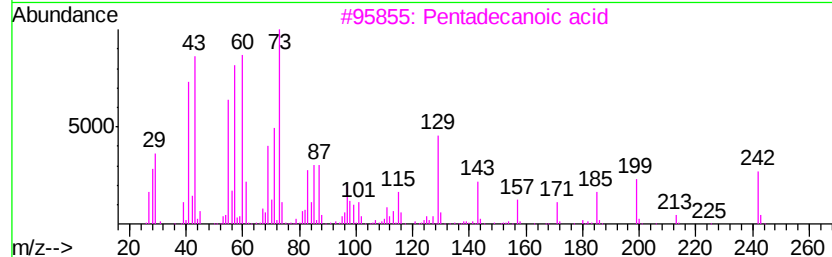
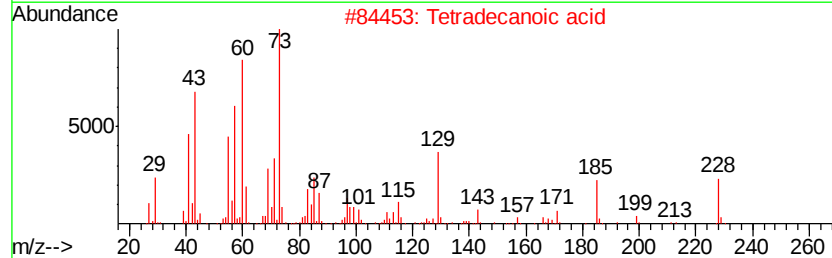
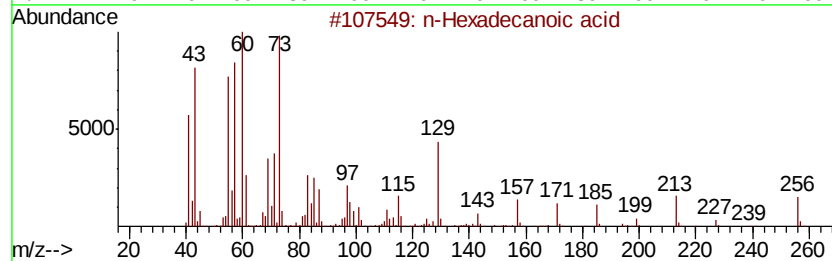
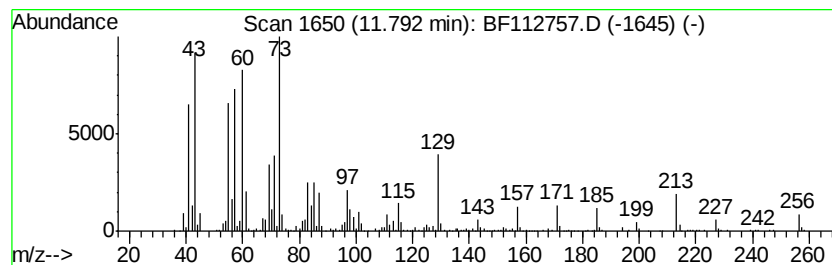
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	12.77 ng	799467	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	91
5		Undecanoic acid	186	C11H22O2	000112-37-8	64



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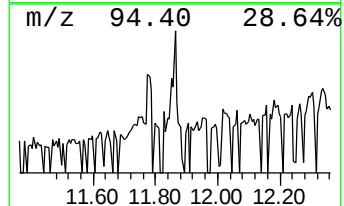
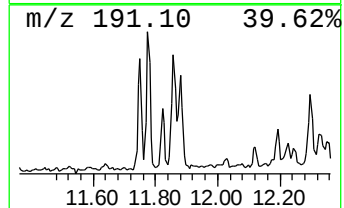
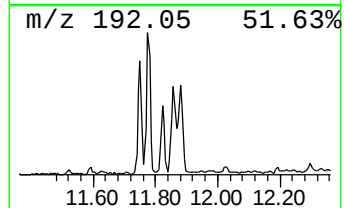
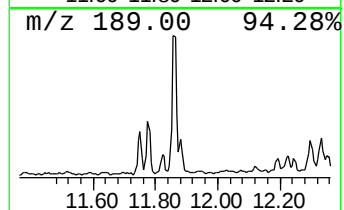
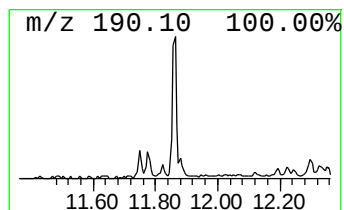
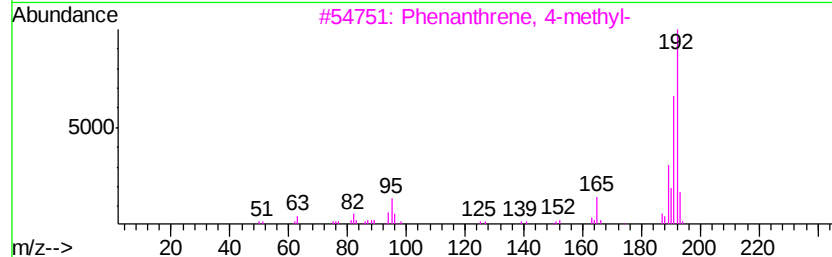
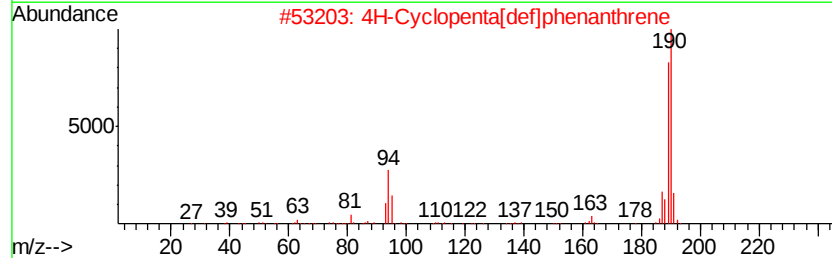
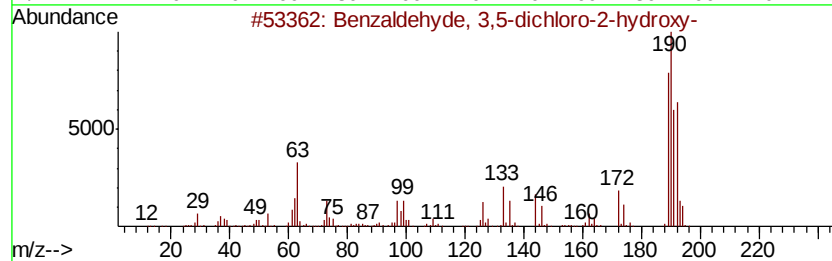
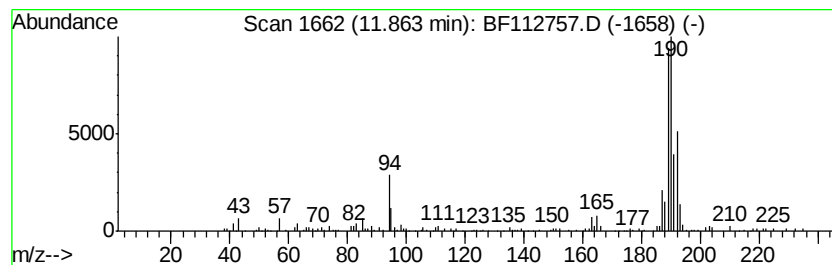
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	2.35 ng	147280	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	80
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	46
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	42



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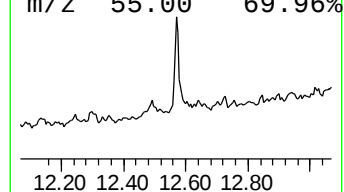
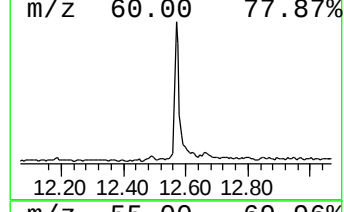
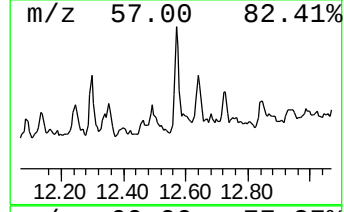
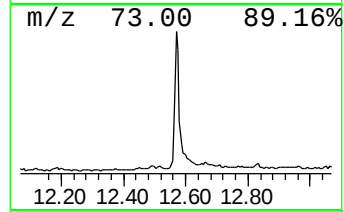
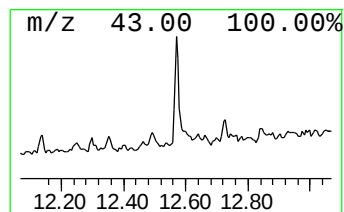
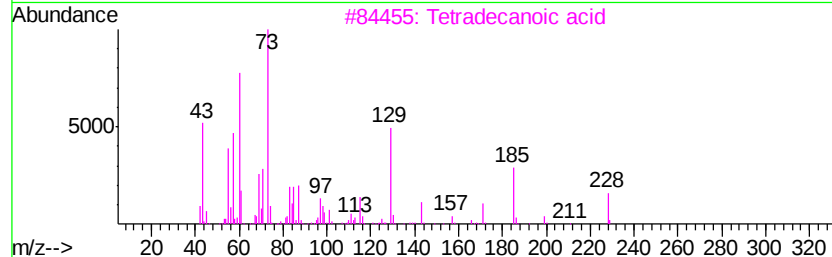
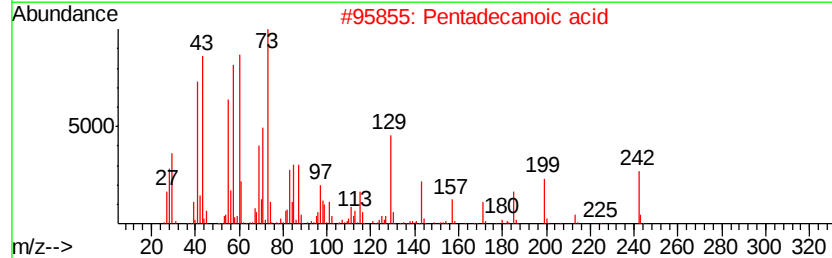
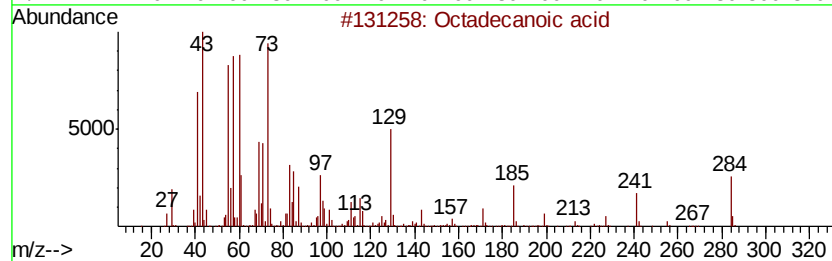
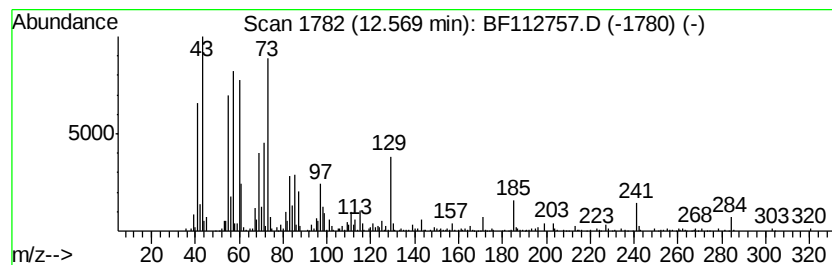
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.57	4.56 ng	426728	Chrysene-d12		13.87
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
4	Nonadecane	268	C19H40	000629-92-5	25
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25



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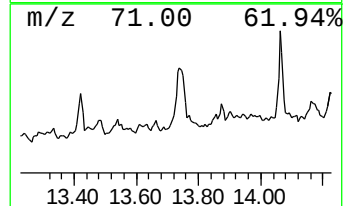
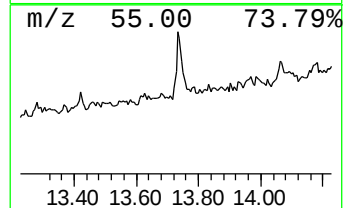
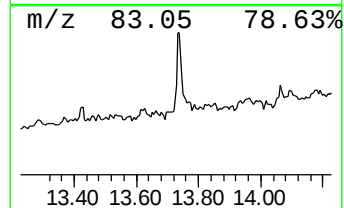
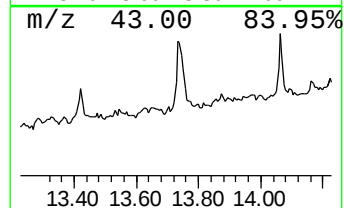
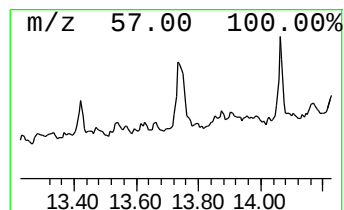
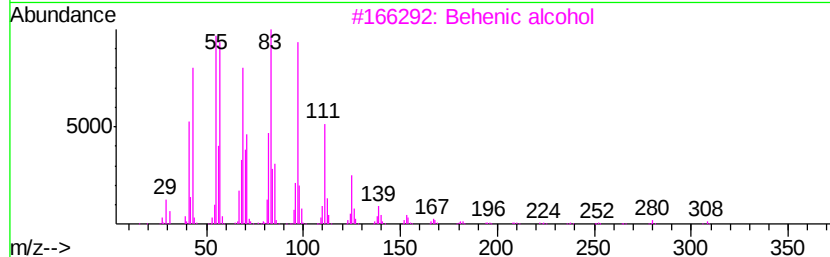
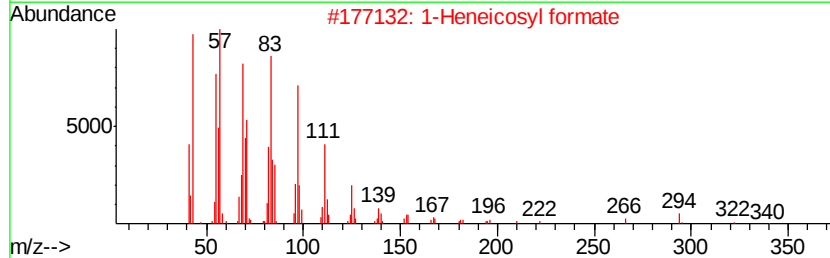
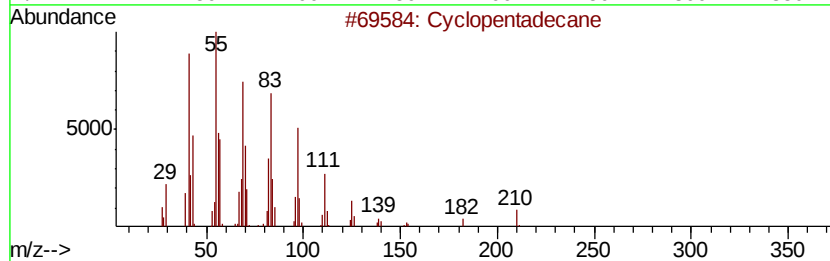
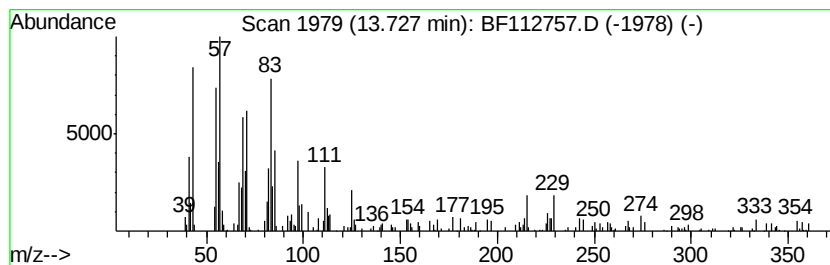
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.73	3.77 ng	352667	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
Data File : BF112757.D
Acq On : 28 Feb 2019 12:54
Operator : JU/SJ
Sample : K1596-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.51	6.51	70.7	ng	3618460	1	6.75	1023570	20.0
n-Hexadecanoic acid	11.79	12.8	ng	799467	4	11.25	1252010	20.0
Benzaldehyde, 3,5...	11.86	2.4	ng	147280	4	11.25	1252010	20.0
Octadecanoic acid	12.57	4.6	ng	426728	5	13.87	1873230	20.0
Cyclopentadecane	13.73	3.8	ng	352667	5	13.87	1873230	20.0